Pergamon

Solid State Communications, Vol. 92, No. 6, pp. 511-513,1994
Elsevier Science Ltd
Printed in Great Britain
0038-1098/94 $7.00+.00

0038-1098(94)00595-8

CHARGE-EXCITATION PICTURE OF Cu NMR KNIGHT SHIFT AND RELAXATION IN $YBa_2Cu_4O_8$ DEDUCED FROM A 3-BAND HUBBARD MODEL

M.V.Eremin, S.V.Varlamov,
D.Brinkmann*, M.Mali*, R.Markendorf* and J.Roos*
Kazan State University, Kazan 420008, Russia
* Physik-Institut, Universität Zürich, Winterthurerstrasse 190,
CH-8057 Zürich, Switzerland

(Received 13 January 1993 by P.Wachter)

(accepted for publication 9 August 1994)

A simplified model of copper hole excitations in the singlet band of $YBa_2Cu_4O_8$ is presented. The starting point is a three-band Hubbard model comprising a Kondo-like exchange between the copper and oxygen holes which gives rise to a new singlet correlated band. This band corresponds to the motion of Zhang-Rice singlets through the antiferromagnetic background of localized copper spins and exhibits a well-developed saddle point of strong copper character. The main contribution to the susceptibility comes from thermally activated copper holes in the extended saddle point of the singlet band. From an idealization of the corresponding density of states we derive formulae for the spin-lattice relaxation time T_1 and the Knight shift K at the Cu(2) site.

1. INTRODUCTION

In high-T_c superconductors (HTSC) the intra-atomic interaction of copper states is very strong compared to usual metals and therefore the Hubbard model provides an adequate description [1]. Many properties of the special quantum fluid in these cuprates manifest themselves in low lying excitations. Thus a great deal of emphasis is given to properties of the microscopic susceptibility which can be studied via the nuclear magnetic resonance (NMR) Knight shift and relaxation.

In our laboratory, we have intensively studied $YBa_2Cu_4O_8$ because of its unique properties such as well defined stoichiometry and thermal stability [2]. In particular we have reported the temperature dependence of the Knight shift for the planar Cu and its anisotropy[3] and the anisotropy and magnetic field dependence of the spin-lattice relaxation in both the normal and superconducting state [3, 4]. These data differ in many respects from those of $YBa_2Cu_3O_7$ reflecting the differences in the electronic structure of both compounds. A summary is given in a recent review by Brinkmann and Mali [5].

In this paper we try to explain Cu Knight shift and relaxation data by thermal excitation of copper holes in the singlet band and a contribution from the spin-degrees of freedom in the lower (or half-filled) Hubbard band. The picture presented here is based on the idea that there is an impurity band [6] in HTSC materials, which corresponds to the motion of Zhang-Rice [7] singlets through the background of the Néel ordered localized copper spins in the lower Hubbard band. Both components contribute to the susceptibility. The singlet-band contribution comes from thermally activated copper holes residing very concentrated in the van Hove singularity. The contribution from the Néel system of localized copper spins is included phenomenologically.

The microscopic basis of this picture is a three-band Hubbard model. From this we derive and present the dispersion of the singlet band. At this stage we leave the microscopic level, keeping only the characteristic features of this band in an idealized density of states. A qualitative description of this situation yields an analytical formula of the susceptibility. On this basis we derive simplified formulae for the Knight shift and spin-lattice relaxation.

From a comparison of these expressions with the experimental data for the Cu(2) site we end up with the conclusion, that in $YBa_2Cu_4O_8$ the low energy physics is governed by a thermal activation of copper holes in the singlet band created by doping. The electronic constellation is such that there is a high density of charge excitations on the transport energy scale. These charge processes show up in a gap-like part of the spin-susceptibility. This point is supported by recent angle resolved photoemission measurements of Abrikosov *et al.* [8]. The possible role of charge excitations has been demonstrated by Lavagna *et al.* [9, 10] in a one-component discription. Our considerations however are based on another microscopic origin of the energy spectrum and on two components in the band, which intersects the Fermi level.

2. MODEL HAMILTONIAN FOR THE SINGLET DISPERSION

We start from a Hubbard Hamiltonian for one copper-oxygen plane in the hole picture where the vacuum state is given by the electronic occupation $|d^{10}p^6>$:

$$H = \varepsilon_d \sum_{i\sigma} \hat{d}^+_{i\sigma}\hat{d}_{i\sigma} + \varepsilon_p \sum_{j\sigma} \hat{p}^+_{j\sigma}\hat{p}_{j\sigma} + \sum_{ij\sigma} t^{pd}_{ij}(\hat{d}^+_{i\sigma}\hat{p}_{j\sigma} + \hat{p}^+_{j\sigma}\hat{d}_{i\sigma}) + \sum_{jj'\sigma} t^{pp}_{jj'}\hat{p}^+_{j\sigma}\hat{p}_{j'\sigma} + J_K \sum_{i\sigma} \psi^+_i \psi_i. \quad (1)$$

Here we use Hubbard operators

$$\hat{d}^+_{i\sigma} = d^+_{i\sigma}(1 - n_{i\bar{\sigma}}), \quad (2)$$

$$n_{i\bar{\sigma}} = d^+_{i\sigma} d_{i\bar{\sigma}}, \quad (3)$$

where $d^+_{i\sigma}$ is a Fermi operator, which creates a local $d_{x^2-y^2}$ hole with spin σ and energy ε_d at the site i. By analogy the local $p_{x(y)}$ states with energy ε_p at an oxygen site j are described by $\hat{p}^+_{j\sigma}$.